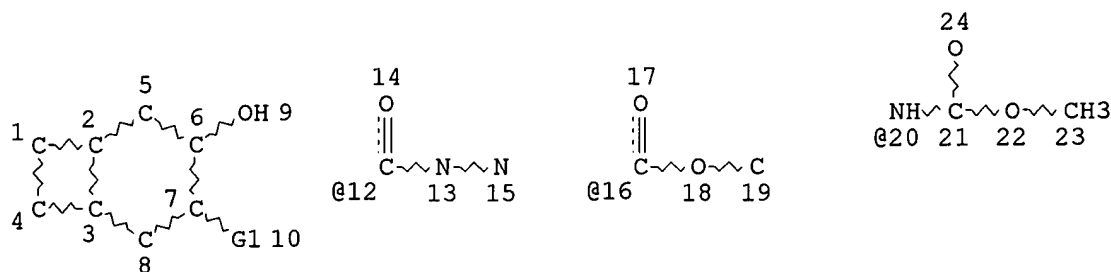


Nyalley, L.
10/656617

10/656617

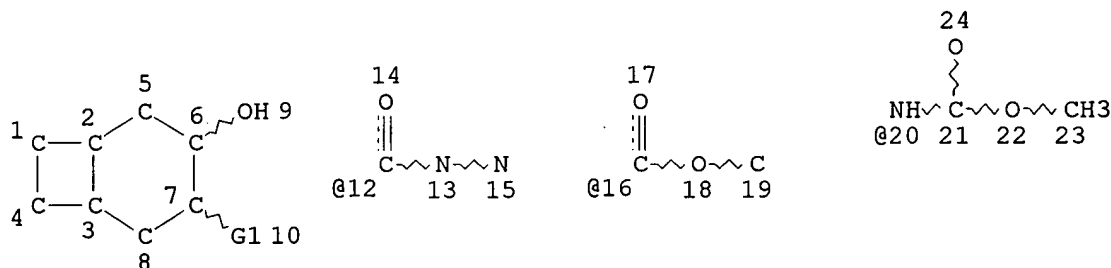
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L16 STR



VAR G1=N/12/16/20
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
L18 19 SEA FILE=REGISTRY SSS FUL L16
L21 STR



VAR G1=N/12/16/20
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
L22 5 SEA FILE=REGISTRY SUB=L18 SSS FUL L21

100.0% PROCESSED 8 ITERATIONS
SEARCH TIME: 00.00.01

5 ANSWERS

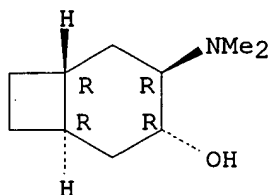
FILE 'CAPLUS' ENTERED AT 14:36:09 ON 09 MAR 2005
L23 3 S L22

L23 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:525681 CAPLUS

Searcher : Shears 571-272-2528

DOCUMENT NUMBER: 79:125681
 TITLE: Conformation and reactivity of [4.n.0]bicyclo systems with trans ring junctions. XIX. Synthesis, conformation, and configuration of 4-Methyl- and 4-halobicyclo[4.2.0]octan-3-ols and -3-ones. Epimerization equilibriums for α -substituted bicyclo[4.2.0]octanones
 AUTHOR(S): Casadevall, E.; Largeau, C.; Moreau, P.; Bouisset, M.
 CORPORATE SOURCE: Ec. Natl. Super. Chim., Paris, Fr.
 SOURCE: Tetrahedron (1973), 29(13), 1865-75
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 AB The conformations and configurations of trans-fused 4-bromo-, 4-chloro-, 4-fluoro-, and 4-methylbicyclo[4.2.0]octan-3-ols and -3-ones, prepared from 3,4-epoxybicyclo[4.2.0]octane and HBr, HCl, Me₂CHNH₃F, and MeLi, resp., were determined by ir, PMR, and uv spectroscopy. The epimerization equils. were determined for the bromo and chloro ketones in AcOH, CCl₄, and dioxane, for the fluoro ketones in CCl₄ and dioxane, and for the Me ketones in CCl₄.
 IT 41441-83-2P 49785-38-8P 49785-45-7P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 41441-83-2 CAPLUS
 CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-, (1 α ,3 α ,4 β ,6 β)- (9CI) (CA INDEX NAME)

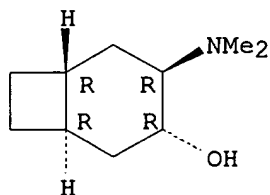
Relative stereochemistry.



RN 49785-38-8 CAPLUS
 CN Butanedioic acid, 2,3-bis(benzoyloxy)-, [R-(R*,R*)]-, compd. with (1 α ,3 α ,4 β ,6 β)-4-(dimethylamino)bicyclo[4.2.0]octan-3-ol (9CI) (CA INDEX NAME)
 CM 1
 CRN 41441-83-2
 CMF C10 H19 N O

Relative stereochemistry.

10/656617

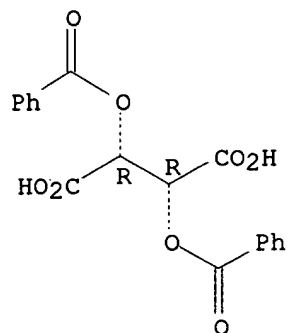


CM 2

CRN 2743-38-6

CMF C18 H14 O8

Absolute stereochemistry.



RN 49785-45-7 CAPLUS

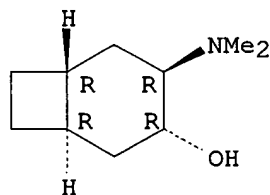
CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-,
(1 α ,3 α ,4 β ,6 β)-, compd. with 2,4,6-trinitrophenol
(9CI) (CA INDEX NAME)

CM 1

CRN 41441-83-2

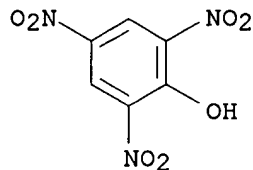
CMF C10 H19 N O

Relative stereochemistry.



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



L23 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:158766 CAPLUS

DOCUMENT NUMBER: 78:158766

TITLE: Conformation and reactivity of trans-fused bicyclo[4.n.0] compounds. XVIII. Spectroscopic study of the conformational equilibrium of trans-fused 4a-dimethylaminobicyclo[4.3.0]nonan-3a-ols and of 4a-dimethylaminobicyclo[4.2.0]octan-3a-ols

AUTHOR(S): Casadevall, Andre; Casadevall, Eliette; Moner, Maryvonne

CORPORATE SOURCE: Ec. Natl. Super. Chim., Paris, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1973), (2) (Pt. 2), 657-62

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

AB The ir spectra of the trans-diaxial-dimethylaminobicyclo[4.3.0]nonanols and of the trans-diaxial-dimethylamino-trans-bicyclo[4.2.0]octanols were observed in the OH stretch region and the free and bound OH bands assigned. The temperature dependence of the OH bands was interpreted in terms of an equilibrium

between a chair conformation, in which H-bonding was intermol., and a flexible conformation in which H-bonding was intramol.; the equilibrium thermodyn. parameters were calculated The disagreement between the NMR and ir

temperature dependencies of the OH peaks in 4a-dimethylaminobicyclo[4.2.0]-octan-3a-ol was discussed.

IT 41441-83-2

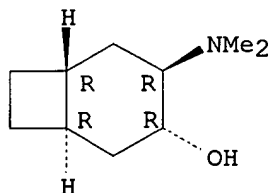
RL: PRP (Properties)

(conformation and hydrogen bonding in, ir and NMR in relation to)

RN 41441-83-2 CAPLUS

CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-, (1 α ,3 α ,4 β ,6 β)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:512248 CAPLUS

DOCUMENT NUMBER: 71:112248

TITLE: Conformation and reactivity of trans-fused bicyclo [4.n.0] derivatives. VII. Elimination reactions of trans-bicyclo [4.2.0] octane

AUTHOR(S): Largeau, Claude; Casadevall, Andre; Casadevall, Eliette

CORPORATE SOURCE: Fac. Sci., Montpellier, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1969), (8), 2734-41

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 71:112248

GI For diagram(s), see printed CA Issue.

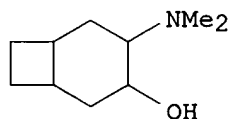
AB trans-Bicyclo[4.2.0]octan-3-ols I are dehydrated (KHSO₄) to give trans-bicyclo[4.2.0]oct-3-ene (II); the I and ZnCl₂ give II-III mixts., where II is the major product. I xanthates are pyrolyzed to give II. I tosylates are treated with NaOMe-MeOH and tert-BuOK-tert-BuOH to give mixts. of II and the alkyl ethers of the I; the 3(a)-tosylate of I and tert-BuOK-tert-BuOH give >99% II.

IT **25137-18-2P 25253-73-0P**

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 25137-18-2 CAPLUS

CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)- (8CI) (CA INDEX NAME)



RN 25253-73-0 CAPLUS

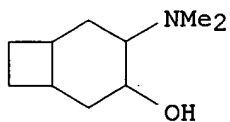
CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 25137-18-2

CMF C10 H19 N O

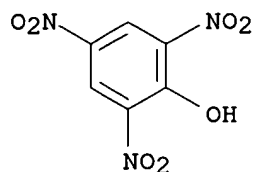
10/656617



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7

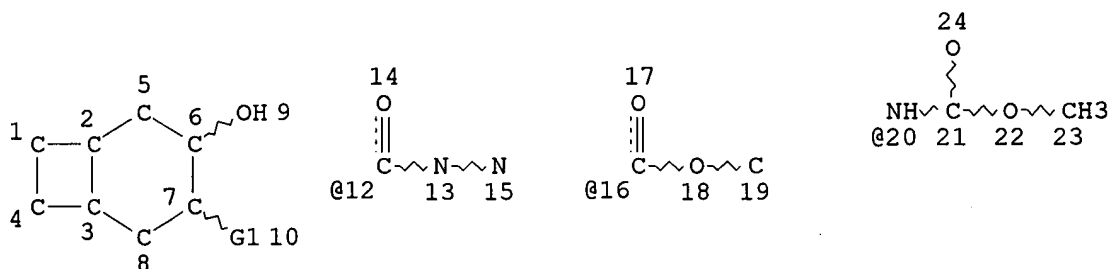


L24 FILE 'CAOLD' ENTERED AT 14:36:34 ON 09 MAR 2005
0 S L22

L25 FILE 'USPATFULL' ENTERED AT 14:36:45 ON 09 MAR 2005
0 S L22

L26 FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 14:36:53 ON 09 MAR 2005
0 S L22

L27 (FILE 'MARPAT' ENTERED AT 14:37:34 ON 09 MAR 2005)
STR



VAR G1=N/12/16/20

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:

ECLEVEL IS LIM ON ALL NODES

Searcher : Shears 571-272-2528

10/656617

ALL RING(S) ARE ISOLATED

L29 1 SEA FILE=MARPAT SSS FUL L27 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 2037 ITERATIONS
SEARCH TIME: 00.00.02

1 ANSWERS

L29 ANSWER 1 OF 1 MARPAT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 136:369713 MARPAT

TITLE: Preparation of 2-cyclohexylmethyl-, cyclohexylamino-, and cyclohexylaminomethylimidazopyridine as NMDA/NR2B antagonists

INVENTOR(S): Thompson, Wayne I.; Claremon, David A.; Munson, Peter M.; Mccauley, John A.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S. Ser. No. 6,291,499.

CODEN: USXXCO

DOCUMENT TYPE: Patent

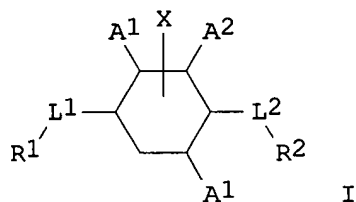
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002055519	A1	20020509	US 2001-861861	20010521
US 6495561	B2	20021217		
US 6291499	B1	20010918	US 2000-696612	20001025
PRIORITY APPLN. INFO.:			US 1999-162714P	19991029
			US 2000-696612	20001025

GI



AB 4-Substituted cyclohexanes substituted in the 1-position with imidazopyridine either directly or through a C1-4 alkyl, C1-4 alkenyl, C1-4 alkynyl, C1-4 alkoxy, amino, amino-C1-4 alkyl, hydroxy-C1-4 alkyl, carbonyl, cyclo-C3-6 alkyl or aminocarbonyl chain represented by general formula [I; R1 = 2-imidazopyridinyl optionally substituted with F, NH2, or HO; R2 = Ph, optionally substituted with one to five substituents, each substituent independently being Cl, F, Br, C1-4 alkyl, CF3, HO, or CO2H; L1, L2 = independently C1-4 alkyl, C1-4 alkoxy, NH2, amino-C1-4 alkyl, hydroxy-C1-4 alkyl, carbonyl, C3-6 cycloalkyl, or aminocarbonyl; A1, A2, A3 are each hydrogen or (i) A1 and A2 form a two carbon bridge or (ii) A1 and A3 form a two carbon bridge; and optionally

Searcher : Shears 571-272-2528

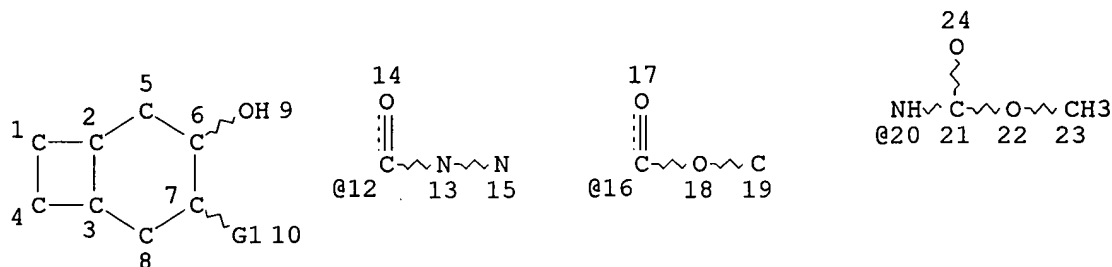
10/656617

substituted with X, wherein X is HO, NH₂, C1-4 alkyl, di(C1-4alkyl)amino, C1-4 alkyl, ester, carbamate, carbonate, or ether] or pharmaceutically acceptable salt thereof are prepared These compds. are effective as N-methyl-D-aspartate (NMDA)/NR2B-subtype receptor antagonists and useful for relieving pain and for the treatment of migraine, depression, anxiety, schizophrenia, Parkinson's disease, or stroke. Thus, Wittig reaction of 4-benzylcyclohexane with 2-benzimidazolylmethyltriphenylphosphonium chloride in the presence of NaH in DMSO gave 2-(4-benzylcyclohexylidenemethyl)-1H-benzimidazole which was hydrogenated over 5% Pt/C in ethanol to give 2-(4-benzylcyclohexylmethyl)-1H-benzimidazole. In a FLIPR (fluorometric imaging plate reader) assay, selected compds. I inhibited NR1A/2B NMDA receptor-mediated Ca²⁺ influx in NR1A/2B NMDA receptor-transfected L(tk) cells with IC₅₀ of <50 μM.

(FILE 'CASREACT' ENTERED AT 14:38:41 ON 09 MAR 2005)

L21

STR



VAR G1=N/12/16/20

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L31 1 SEA FILE=CASREACT SSS FUL L21 (1 REACTIONS)

100.0% DONE 4203 VERIFIED

1 HIT RXNS

1 DOCS

SEARCH TIME: 00.00.01

L31 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 71:112248 CASREACT

TITLE: Conformation and reactivity of trans-fused bicyclo [4.n.0] derivatives. VII. Elimination reactions of trans-bicyclo [4.2.0] octane

AUTHOR(S): Largeau, Claude; Casadevall, Andre; Casadevall, Eliette

CORPORATE SOURCE: Fac. Sci., Montpellier, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1969), (8), 2734-41

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

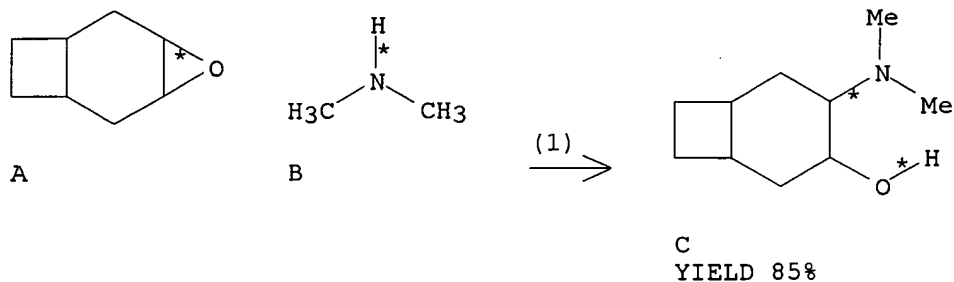
GI For diagram(s), see printed CA Issue.

Searcher : Shears 571-272-2528

10/656617

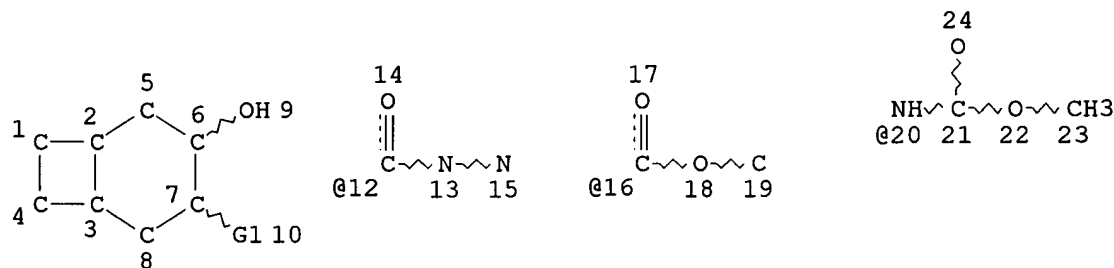
AB trans-Bicyclo[4.2.0]octan-3-ols I are dehydrated (KHSO4) to give trans-bicyclo[4.2.0]oct-3-ene (II); the I and ZnCl2 give II-III mixts., where II is the major product. I xanthates are pyrolyzed to give II. I tosylates are treated with NaOMe-MeOH and tert-BuOK-tert-BuOH to give mixts. of II and the alkyl ethers of the I; the 3(a)-tosylate of I and tert-BuOK-tert-BuOH give >99% II.

RX(1) OF 1 A + B ==> C



RX(1) RCT A 286-59-9, B 124-40-3
 PRO C 25137-18-2
 SOL 7732-18-5 Water
 NTE Classification: Epoxide cleavage; C-Amination; # Conditions: H2O
 120 deg 15h; # Comments: trans reactant

(FILE 'DJSMDs, CHEMINFORMRX' ENTERED AT 14:39:40 ON 09 MAR 2005)
 L21 STR



VAR G1=N/12/16/20
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

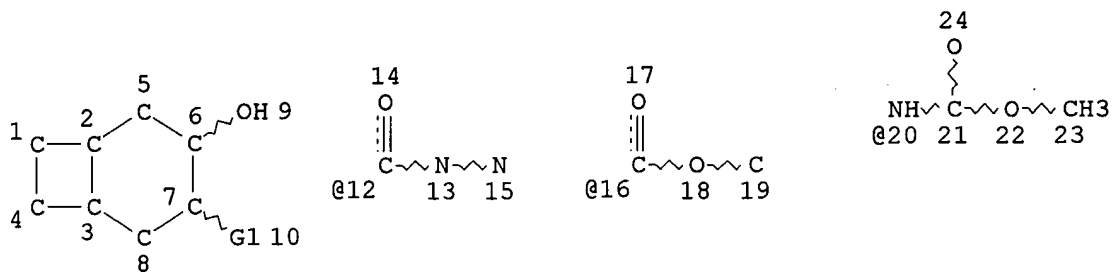
GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
 L32 0 SEA L21

FILE 'MARPATPREV' ENTERED AT 14:44:55 ON 09 MAR 2005
 L27 STR

Searcher : Shears 571-272-2528

10/656617



VAR G1=N/12/16/20
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

L33 0 SEA FILE=MARPATPREV SSS FUL L27 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 4 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FILE 'HOME' ENTERED AT 14:45:16 ON 09 MAR 2005